wwPDB X-ray Structure Validation Summary Report (i)

Jun 17, 2024 – 10:30 PM EDT

PDB ID	:	5XGO
Title	:	The Ferritin E-Domain: Toward Understanding Its Role in Protein Cage Assembly Through the Crystal Structure of a Maxi-/Mini-Ferritin Chimera
Authors	:	Cornell, T.A.; Srivastava, Y.; Jauch, R.; Fan, R.; Orner, B.P.
Deposited on	:	2017-04-14
Resolution	:	1.99 Å(reported)

The following versions of software and data (see references (i)) were used in the production of this report:

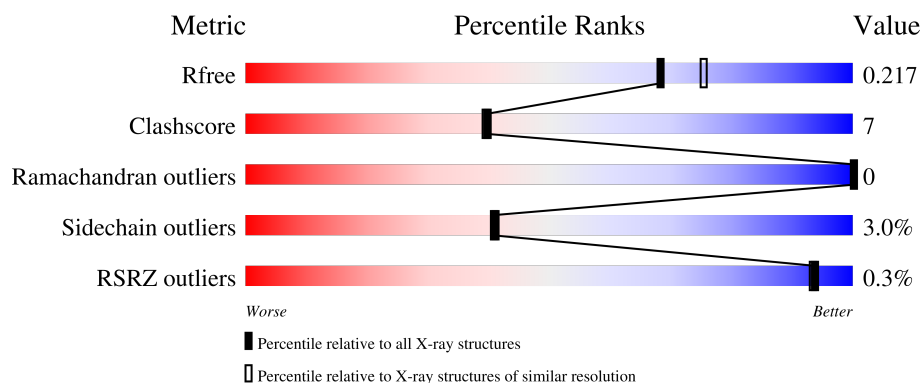|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1   Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.99 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.

Metric	Percentile Ranks	Value
Rfree		0.217
Clashscore		7
Ramachandran outliers		0
Sidechain outliers		3.0%
RSRZ outliers		0.3%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	200	68% 7% • 22%
1	B	200	64% 11% • • 22%
1	C	200	68% 8% • 22%
1	D	200	66% 10% • 22%
1	E	200	60% 17% 22%

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Mol	Chain	Length	Quality of chain
1	F	200	66% 10% 22%
1	G	200	% 66% 8% 22%
1	H	200	68% 6% 22%
1	I	200	66% 10% 22%
1	J	200	68% 8% 22%
1	K	200	62% 12% 22%
1	L	200	% 68% 8% 22%

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 16563 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA protection during starvation protein,Bacterioferritin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	155	Total	C	N	O	S	0	0	0
			1227	773	214	236	4			
1	B	156	Total	C	N	O	S	0	0	0
			1235	777	216	238	4			
1	C	155	Total	C	N	O	S	0	0	0
			1227	773	214	236	4			
1	D	156	Total	C	N	O	S	0	0	0
			1235	777	216	238	4			
1	E	155	Total	C	N	O	S	0	0	0
			1227	773	214	236	4			
1	F	156	Total	C	N	O	S	0	0	0
			1235	777	216	238	4			
1	G	156	Total	C	N	O	S	0	0	0
			1235	777	216	238	4			
1	H	156	Total	C	N	O	S	0	0	0
			1235	777	216	238	4			
1	I	156	Total	C	N	O	S	0	0	0
			1235	777	216	238	4			
1	J	155	Total	C	N	O	S	0	0	0
			1227	773	214	236	4			
1	K	156	Total	C	N	O	S	0	0	0
			1235	777	216	238	4			
1	L	155	Total	C	N	O	S	0	0	0
			1227	773	214	236	4			

There are 192 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	expression tag	UNP P0ABT2
A	-12	ALA	-	expression tag	UNP P0ABT2
A	-11	HIS	-	expression tag	UNP P0ABT2
A	-10	HIS	-	expression tag	UNP P0ABT2
A	-9	HIS	-	expression tag	UNP P0ABT2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	HIS	-	expression tag	UNP P0ABT2
A	-7	HIS	-	expression tag	UNP P0ABT2
A	-6	HIS	-	expression tag	UNP P0ABT2
A	-5	VAL	-	expression tag	UNP P0ABT2
A	-4	ASP	-	expression tag	UNP P0ABT2
A	-3	ASP	-	expression tag	UNP P0ABT2
A	-2	ASP	-	expression tag	UNP P0ABT2
A	-1	ASP	-	expression tag	UNP P0ABT2
A	0	LYS	-	expression tag	UNP P0ABT2
A	164	CYS	-	linker	UNP P0ABT2
A	165	ASN	-	linker	UNP P0ABT2
B	-13	MET	-	expression tag	UNP P0ABT2
B	-12	ALA	-	expression tag	UNP P0ABT2
B	-11	HIS	-	expression tag	UNP P0ABT2
B	-10	HIS	-	expression tag	UNP P0ABT2
B	-9	HIS	-	expression tag	UNP P0ABT2
B	-8	HIS	-	expression tag	UNP P0ABT2
B	-7	HIS	-	expression tag	UNP P0ABT2
B	-6	HIS	-	expression tag	UNP P0ABT2
B	-5	VAL	-	expression tag	UNP P0ABT2
B	-4	ASP	-	expression tag	UNP P0ABT2
B	-3	ASP	-	expression tag	UNP P0ABT2
B	-2	ASP	-	expression tag	UNP P0ABT2
B	-1	ASP	-	expression tag	UNP P0ABT2
B	0	LYS	-	expression tag	UNP P0ABT2
B	164	CYS	-	linker	UNP P0ABT2
B	165	ASN	-	linker	UNP P0ABT2
C	-13	MET	-	expression tag	UNP P0ABT2
C	-12	ALA	-	expression tag	UNP P0ABT2
C	-11	HIS	-	expression tag	UNP P0ABT2
C	-10	HIS	-	expression tag	UNP P0ABT2
C	-9	HIS	-	expression tag	UNP P0ABT2
C	-8	HIS	-	expression tag	UNP P0ABT2
C	-7	HIS	-	expression tag	UNP P0ABT2
C	-6	HIS	-	expression tag	UNP P0ABT2
C	-5	VAL	-	expression tag	UNP P0ABT2
C	-4	ASP	-	expression tag	UNP P0ABT2
C	-3	ASP	-	expression tag	UNP P0ABT2
C	-2	ASP	-	expression tag	UNP P0ABT2
C	-1	ASP	-	expression tag	UNP P0ABT2
C	0	LYS	-	expression tag	UNP P0ABT2
C	164	CYS	-	linker	UNP P0ABT2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	165	ASN	-	linker	UNP P0ABT2
D	-13	MET	-	expression tag	UNP P0ABT2
D	-12	ALA	-	expression tag	UNP P0ABT2
D	-11	HIS	-	expression tag	UNP P0ABT2
D	-10	HIS	-	expression tag	UNP P0ABT2
D	-9	HIS	-	expression tag	UNP P0ABT2
D	-8	HIS	-	expression tag	UNP P0ABT2
D	-7	HIS	-	expression tag	UNP P0ABT2
D	-6	HIS	-	expression tag	UNP P0ABT2
D	-5	VAL	-	expression tag	UNP P0ABT2
D	-4	ASP	-	expression tag	UNP P0ABT2
D	-3	ASP	-	expression tag	UNP P0ABT2
D	-2	ASP	-	expression tag	UNP P0ABT2
D	-1	ASP	-	expression tag	UNP P0ABT2
D	0	LYS	-	expression tag	UNP P0ABT2
D	164	CYS	-	linker	UNP P0ABT2
D	165	ASN	-	linker	UNP P0ABT2
E	-13	MET	-	expression tag	UNP P0ABT2
E	-12	ALA	-	expression tag	UNP P0ABT2
E	-11	HIS	-	expression tag	UNP P0ABT2
E	-10	HIS	-	expression tag	UNP P0ABT2
E	-9	HIS	-	expression tag	UNP P0ABT2
E	-8	HIS	-	expression tag	UNP P0ABT2
E	-7	HIS	-	expression tag	UNP P0ABT2
E	-6	HIS	-	expression tag	UNP P0ABT2
E	-5	VAL	-	expression tag	UNP P0ABT2
E	-4	ASP	-	expression tag	UNP P0ABT2
E	-3	ASP	-	expression tag	UNP P0ABT2
E	-2	ASP	-	expression tag	UNP P0ABT2
E	-1	ASP	-	expression tag	UNP P0ABT2
E	0	LYS	-	expression tag	UNP P0ABT2
E	164	CYS	-	linker	UNP P0ABT2
E	165	ASN	-	linker	UNP P0ABT2
F	-13	MET	-	expression tag	UNP P0ABT2
F	-12	ALA	-	expression tag	UNP P0ABT2
F	-11	HIS	-	expression tag	UNP P0ABT2
F	-10	HIS	-	expression tag	UNP P0ABT2
F	-9	HIS	-	expression tag	UNP P0ABT2
F	-8	HIS	-	expression tag	UNP P0ABT2
F	-7	HIS	-	expression tag	UNP P0ABT2
F	-6	HIS	-	expression tag	UNP P0ABT2
F	-5	VAL	-	expression tag	UNP P0ABT2

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-4	ASP	-	expression tag	UNP P0ABT2
F	-3	ASP	-	expression tag	UNP P0ABT2
F	-2	ASP	-	expression tag	UNP P0ABT2
F	-1	ASP	-	expression tag	UNP P0ABT2
F	0	LYS	-	expression tag	UNP P0ABT2
F	164	CYS	-	linker	UNP P0ABT2
F	165	ASN	-	linker	UNP P0ABT2
G	-13	MET	-	expression tag	UNP P0ABT2
G	-12	ALA	-	expression tag	UNP P0ABT2
G	-11	HIS	-	expression tag	UNP P0ABT2
G	-10	HIS	-	expression tag	UNP P0ABT2
G	-9	HIS	-	expression tag	UNP P0ABT2
G	-8	HIS	-	expression tag	UNP P0ABT2
G	-7	HIS	-	expression tag	UNP P0ABT2
G	-6	HIS	-	expression tag	UNP P0ABT2
G	-5	VAL	-	expression tag	UNP P0ABT2
G	-4	ASP	-	expression tag	UNP P0ABT2
G	-3	ASP	-	expression tag	UNP P0ABT2
G	-2	ASP	-	expression tag	UNP P0ABT2
G	-1	ASP	-	expression tag	UNP P0ABT2
G	0	LYS	-	expression tag	UNP P0ABT2
G	164	CYS	-	linker	UNP P0ABT2
G	165	ASN	-	linker	UNP P0ABT2
H	-13	MET	-	expression tag	UNP P0ABT2
H	-12	ALA	-	expression tag	UNP P0ABT2
H	-11	HIS	-	expression tag	UNP P0ABT2
H	-10	HIS	-	expression tag	UNP P0ABT2
H	-9	HIS	-	expression tag	UNP P0ABT2
H	-8	HIS	-	expression tag	UNP P0ABT2
H	-7	HIS	-	expression tag	UNP P0ABT2
H	-6	HIS	-	expression tag	UNP P0ABT2
H	-5	VAL	-	expression tag	UNP P0ABT2
H	-4	ASP	-	expression tag	UNP P0ABT2
H	-3	ASP	-	expression tag	UNP P0ABT2
H	-2	ASP	-	expression tag	UNP P0ABT2
H	-1	ASP	-	expression tag	UNP P0ABT2
H	0	LYS	-	expression tag	UNP P0ABT2
H	164	CYS	-	linker	UNP P0ABT2
H	165	ASN	-	linker	UNP P0ABT2
I	-13	MET	-	expression tag	UNP P0ABT2
I	-12	ALA	-	expression tag	UNP P0ABT2
I	-11	HIS	-	expression tag	UNP P0ABT2

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Chain	Residue	Modelled	Actual	Comment	Reference
I	-10	HIS	-	expression tag	UNP P0ABT2
I	-9	HIS	-	expression tag	UNP P0ABT2
I	-8	HIS	-	expression tag	UNP P0ABT2
I	-7	HIS	-	expression tag	UNP P0ABT2
I	-6	HIS	-	expression tag	UNP P0ABT2
I	-5	VAL	-	expression tag	UNP P0ABT2
I	-4	ASP	-	expression tag	UNP P0ABT2
I	-3	ASP	-	expression tag	UNP P0ABT2
I	-2	ASP	-	expression tag	UNP P0ABT2
I	-1	ASP	-	expression tag	UNP P0ABT2
I	0	LYS	-	expression tag	UNP P0ABT2
I	164	CYS	-	linker	UNP P0ABT2
I	165	ASN	-	linker	UNP P0ABT2
J	-13	MET	-	expression tag	UNP P0ABT2
J	-12	ALA	-	expression tag	UNP P0ABT2
J	-11	HIS	-	expression tag	UNP P0ABT2
J	-10	HIS	-	expression tag	UNP P0ABT2
J	-9	HIS	-	expression tag	UNP P0ABT2
J	-8	HIS	-	expression tag	UNP P0ABT2
J	-7	HIS	-	expression tag	UNP P0ABT2
J	-6	HIS	-	expression tag	UNP P0ABT2
J	-5	VAL	-	expression tag	UNP P0ABT2
J	-4	ASP	-	expression tag	UNP P0ABT2
J	-3	ASP	-	expression tag	UNP P0ABT2
J	-2	ASP	-	expression tag	UNP P0ABT2
J	-1	ASP	-	expression tag	UNP P0ABT2
J	0	LYS	-	expression tag	UNP P0ABT2
J	164	CYS	-	linker	UNP P0ABT2
J	165	ASN	-	linker	UNP P0ABT2
K	-13	MET	-	expression tag	UNP P0ABT2
K	-12	ALA	-	expression tag	UNP P0ABT2
K	-11	HIS	-	expression tag	UNP P0ABT2
K	-10	HIS	-	expression tag	UNP P0ABT2
K	-9	HIS	-	expression tag	UNP P0ABT2
K	-8	HIS	-	expression tag	UNP P0ABT2
K	-7	HIS	-	expression tag	UNP P0ABT2
K	-6	HIS	-	expression tag	UNP P0ABT2
K	-5	VAL	-	expression tag	UNP P0ABT2
K	-4	ASP	-	expression tag	UNP P0ABT2
K	-3	ASP	-	expression tag	UNP P0ABT2
K	-2	ASP	-	expression tag	UNP P0ABT2
K	-1	ASP	-	expression tag	UNP P0ABT2

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Chain	Residue	Modelled	Actual	Comment	Reference
K	0	LYS	-	expression tag	UNP P0ABT2
K	164	CYS	-	linker	UNP P0ABT2
K	165	ASN	-	linker	UNP P0ABT2
L	-13	MET	-	expression tag	UNP P0ABT2
L	-12	ALA	-	expression tag	UNP P0ABT2
L	-11	HIS	-	expression tag	UNP P0ABT2
L	-10	HIS	-	expression tag	UNP P0ABT2
L	-9	HIS	-	expression tag	UNP P0ABT2
L	-8	HIS	-	expression tag	UNP P0ABT2
L	-7	HIS	-	expression tag	UNP P0ABT2
L	-6	HIS	-	expression tag	UNP P0ABT2
L	-5	VAL	-	expression tag	UNP P0ABT2
L	-4	ASP	-	expression tag	UNP P0ABT2
L	-3	ASP	-	expression tag	UNP P0ABT2
L	-2	ASP	-	expression tag	UNP P0ABT2
L	-1	ASP	-	expression tag	UNP P0ABT2
L	0	LYS	-	expression tag	UNP P0ABT2
L	164	CYS	-	linker	UNP P0ABT2
L	165	ASN	-	linker	UNP P0ABT2

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Cl 1	0	0
2	H	1	Total 1	Cl 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	129	Total 129	O 129	0	0
3	B	171	Total 171	O 171	0	0
3	C	158	Total 158	O 158	0	0
3	D	152	Total 152	O 152	0	0
3	E	173	Total 173	O 173	0	0
3	F	151	Total 151	O 151	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	141	Total 141	O 141	0	0
3	H	156	Total 156	O 156	0	0
3	I	148	Total 148	O 148	0	0
3	J	113	Total 113	O 113	0	0
3	K	161	Total 161	O 161	0	0
3	L	128	Total 128	O 128	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

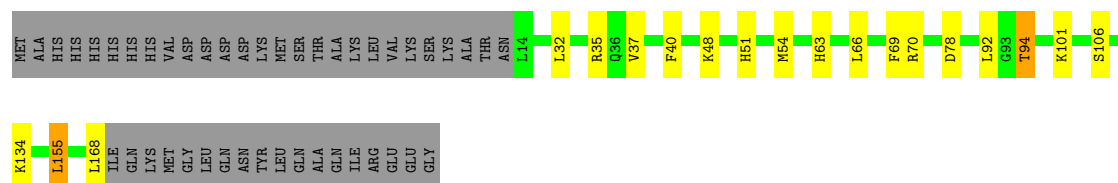- Molecule 1: DNA protection during starvation protein,Bacterioferritin

Chain A:
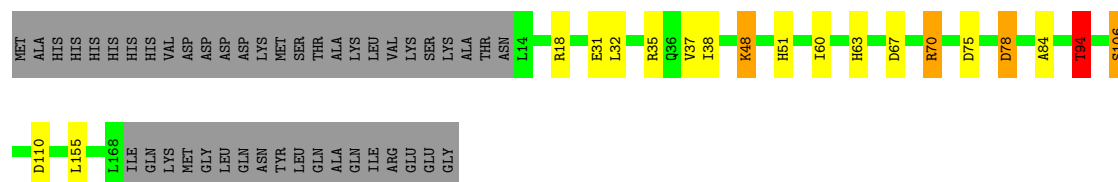
- Molecule 1: DNA protection during starvation protein,Bacterioferritin

Chain B:
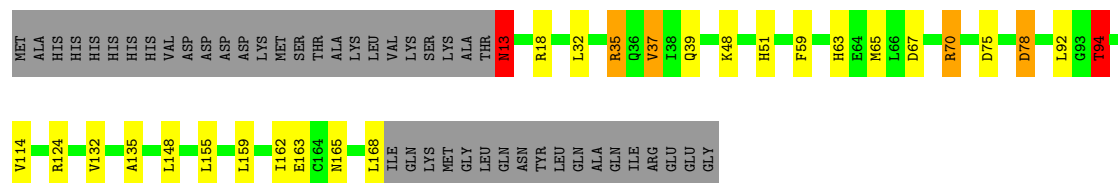
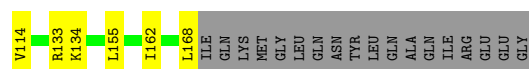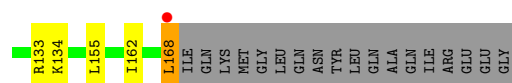- Molecule 1: DNA protection during starvation protein,Bacterioferritin

Chain C:

- Molecule 1: DNA protection during starvation protein,Bacterioferritin
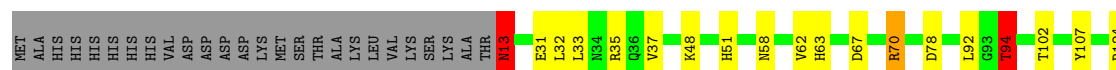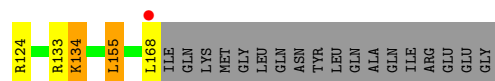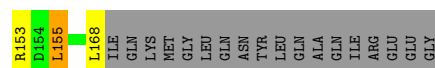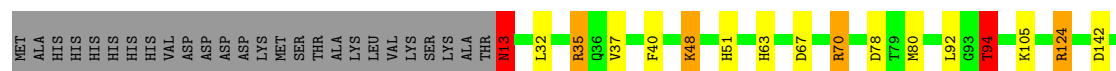
Chain D:

V114 R133 K134 L155 I162 L168 ILE GLN LYS MET GLY LEU GLN ASN TYR LEU GLN ALA GLN ILE ARG GLU GLU GLY

• Molecule 1: DNA protection during starvation protein,Bacterioferritin

Chain E:

60%   17%   22%

MET ALA HIS HIS HIS HIS HIS VAL ASP ASP ASP LYS MET SER THR ALA LYS LEU VAL LYS SER LYS ALA THR ASN L14 R18 K26 E31 R35 Q36 V37 I38 Q39 L43 S44 T47 K48 H51 V62 H63 D67 R70 L73 I74 D75 H76

L77 D78 T79 M80 L92 T102 P103 A122 K134 A139 T144 A145 L148 L155 L159 W160 F161 I162 E163 L168 ILE GLN LYS MET GLY LEU GLN ASN TYR LEU GLN ALA GLN ILE ARG GLU GLU GLY

• Molecule 1: DNA protection during starvation protein,Bacterioferritin

Chain F:

66%   10%   ··   22%

MET ALA HIS HIS HIS HIS HIS VAL ASP ASP ASP LYS MET SER THR ALA LYS LEU VAL LYS SER LYS ALA THR N13 E31 L32 L33 N34 R35 Q36 V37 K48 H51 N58 V62 H63 D67 R70 D78 L92 G93 T94 T102 Y107 R124

R133 K134 L155 I162 L168 ILE GLN LYS MET GLY LEU GLN ASN TYR LEU GLN ALA GLN ILE ARG GLU GLU GLY

• Molecule 1: DNA protection during starvation protein,Bacterioferritin

Chain G:

%

66%   8%   ·   22%

MET ALA HIS HIS HIS HIS HIS VAL ASP ASP ASP LYS MET SER THR ALA LYS LEU VAL LYS SER LYS ALA THR N13 L32 R35 Q36 V37 F40 T47 K48 Q49 A50 H51 H63 D67 R70 D78 Q86 I94 V97 S100 K105

R124 R133 K134 L155 L168 ILE GLN LYS MET GLY LEU GLN ASN TYR LEU GLN ALA GLN ILE ARG GLU GLU GLY

• Molecule 1: DNA protection during starvation protein,Bacterioferritin

Chain H:

68%   6%   ··   22%

MET ALA HIS HIS HIS HIS HIS VAL ASP ASP ASP LYS MET SER THR ALA LYS LEU VAL LYS SER LYS ALA THR N13 L32 R35 Q36 V37 F40 K48 H51 H63 D67 R70 D78 T79 M80 L92 G93 T94 K105 R124 D142

R153 D154 L155 L168 ILE GLN LYS MET GLY LEU GLN ASN TYR LEU GLN ALA GLN ILE ARG GLU GLU GLY

• Molecule 1: DNA protection during starvation protein,Bacterioferritin

Chain I:
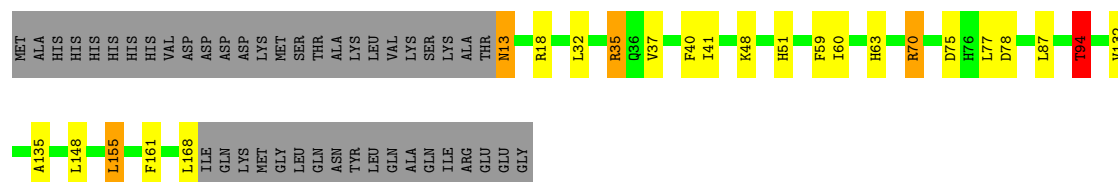
66%   10%   ·   22%

• Molecule 1: DNA protection during starvation protein,Bacterioferritin

Chain J:

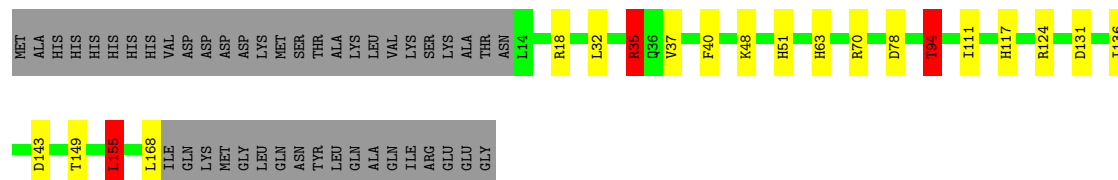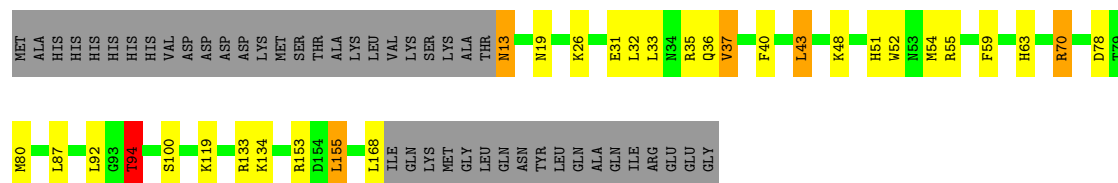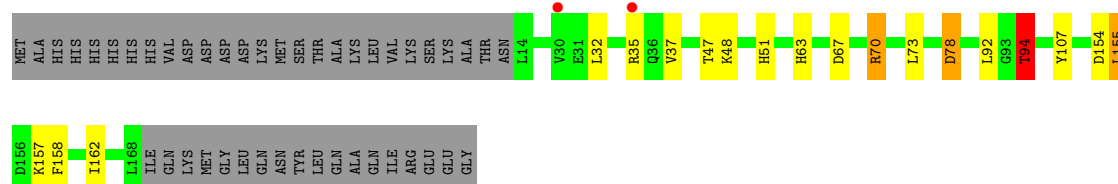• Molecule 1: DNA protection during starvation protein,Bacterioferritin

Chain K:

• Molecule 1: DNA protection during starvation protein,Bacterioferritin

Chain L:

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	103.14Å 104.72Å 207.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.76 – 1.99 46.76 – 1.99	Depositor EDS
% Data completeness (in resolution range)	92.3 (46.76-1.99) 91.8 (46.76-1.99)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.50 (at 1.98Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.179 , 0.207 0.188 , 0.217	Depositor DCC
R_{free} test set	7167 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	28.3	Xtriage
Anisotropy	0.023	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 34.9	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.016 for k,h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	16563	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.49% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	A	1.06	4/1245 (0.3%)	1.04	10/1687 (0.6%)
1	B	0.95	1/1253 (0.1%)	1.02	12/1698 (0.7%)
1	C	0.98	2/1245 (0.2%)	1.04	8/1687 (0.5%)
1	D	0.98	2/1253 (0.2%)	1.06	11/1698 (0.6%)
1	E	0.96	1/1245 (0.1%)	1.13	10/1687 (0.6%)
1	F	0.93	2/1253 (0.2%)	1.07	11/1698 (0.6%)
1	G	0.94	2/1253 (0.2%)	1.06	11/1698 (0.6%)
1	H	0.92	1/1253 (0.1%)	1.05	9/1698 (0.5%)
1	I	0.90	1/1253 (0.1%)	1.08	12/1698 (0.7%)
1	J	0.78	1/1245 (0.1%)	1.03	11/1687 (0.7%)
1	K	0.90	2/1253 (0.2%)	1.02	8/1698 (0.5%)
1	L	0.79	0/1245	0.96	8/1687 (0.5%)
All	All	0.93	19/14996 (0.1%)	1.05	121/20321 (0.6%)

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	106	SER	CB-OG	-10.46	1.28	1.42
1	A	106	SER	CB-OG	-10.37	1.28	1.42
1	B	94	THR	CB-CG2	-7.52	1.27	1.52
1	K	100	SER	CB-OG	-6.75	1.33	1.42
1	K	94	THR	CB-CG2	-6.61	1.30	1.52

The worst 5 of 121 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	35	ARG	NE-CZ-NH1	14.99	127.80	120.30
1	E	35	ARG	NE-CZ-NH2	-14.86	112.87	120.30
1	G	155	LEU	CB-CG-CD1	12.91	132.94	111.00
1	I	155	LEU	CB-CG-CD1	12.74	132.66	111.00
1	F	155	LEU	CB-CG-CD1	12.56	132.36	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1227	0	1228	12	0
1	B	1235	0	1234	24	0
1	C	1227	0	1228	10	0
1	D	1235	0	1234	19	0
1	E	1227	0	1228	30	0
1	F	1235	0	1234	16	0
1	G	1235	0	1234	13	0
1	H	1235	0	1234	18	0
1	I	1235	0	1234	18	0
1	J	1227	0	1228	13	0
1	K	1235	0	1234	25	0
1	L	1227	0	1228	17	0
2	A	1	0	0	0	0
2	H	1	0	0	0	0
3	A	129	0	0	7	0
3	B	171	0	0	22	0
3	C	158	0	0	7	0
3	D	152	0	0	15	0
3	E	173	0	0	34	0
3	F	151	0	0	11	0
3	G	141	0	0	9	0
3	H	156	0	0	16	0
3	I	148	0	0	18	0
3	J	113	0	0	14	0
3	K	161	0	0	22	0
3	L	128	0	0	13	0
All	All	16563	0	14778	215	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 215 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:75:ASP:HB2	3:E:329:HOH:O	1.46	1.14
1:E:47:THR:OG1	3:E:201:HOH:O	1.76	1.03
1:E:134:LYS:NZ	3:E:202:HOH:O	1.79	0.98
3:B:281:HOH:O	1:G:78:ASP:HB2	1.60	0.98
1:I:75:ASP:HB2	3:I:300:HOH:O	1.61	0.97

There are no symmetry-related clashes.

5.3   Torsion angles (i)

5.3.1   Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	153/200 (76%)	152 (99%)	1 (1%)	0	100	100
1	B	154/200 (77%)	152 (99%)	2 (1%)	0	100	100
1	C	153/200 (76%)	152 (99%)	1 (1%)	0	100	100
1	D	154/200 (77%)	152 (99%)	2 (1%)	0	100	100
1	E	153/200 (76%)	152 (99%)	1 (1%)	0	100	100
1	F	154/200 (77%)	153 (99%)	1 (1%)	0	100	100
1	G	154/200 (77%)	153 (99%)	1 (1%)	0	100	100
1	H	154/200 (77%)	153 (99%)	1 (1%)	0	100	100
1	I	154/200 (77%)	152 (99%)	2 (1%)	0	100	100
1	J	153/200 (76%)	152 (99%)	1 (1%)	0	100	100
1	K	154/200 (77%)	153 (99%)	1 (1%)	0	100	100
1	L	153/200 (76%)	151 (99%)	2 (1%)	0	100	100
All	All	1843/2400 (77%)	1827 (99%)	16 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	133/172 (77%)	129 (97%)	4 (3%)	41	41
1	B	134/172 (78%)	129 (96%)	5 (4%)	34	32
1	C	133/172 (77%)	130 (98%)	3 (2%)	50	53
1	D	134/172 (78%)	129 (96%)	5 (4%)	34	32
1	E	133/172 (77%)	132 (99%)	1 (1%)	81	86
1	F	134/172 (78%)	130 (97%)	4 (3%)	41	41
1	G	134/172 (78%)	129 (96%)	5 (4%)	34	32
1	H	134/172 (78%)	130 (97%)	4 (3%)	41	41
1	I	134/172 (78%)	130 (97%)	4 (3%)	41	41
1	J	133/172 (77%)	128 (96%)	5 (4%)	33	31
1	K	134/172 (78%)	128 (96%)	6 (4%)	27	24
1	L	133/172 (77%)	131 (98%)	2 (2%)	65	69
All	All	1603/2064 (78%)	1555 (97%)	48 (3%)	41	41

5 of 48 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	35	ARG
1	J	35	ARG
1	H	94	THR
1	I	35	ARG
1	J	94	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	39	GLN
1	H	51	HIS
1	K	112	HIS
1	H	39	GLN

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Mol	Chain	Res	Type
1	I	39	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	155/200 (77%)	-0.27	0	100	100	20, 26, 38, 49	0
1	B	156/200 (78%)	-0.42	0	100	100	21, 28, 42, 54	0
1	C	155/200 (77%)	-0.27	0	100	100	20, 27, 41, 50	0
1	D	156/200 (78%)	-0.23	0	100	100	22, 29, 43, 50	0
1	E	155/200 (77%)	-0.31	0	100	100	21, 26, 40, 51	0
1	F	156/200 (78%)	-0.36	1 (0%)	89	88	23, 29, 44, 53	0
1	G	156/200 (78%)	-0.15	2 (1%)	77	76	22, 29, 48, 59	0
1	H	156/200 (78%)	-0.23	0	100	100	23, 30, 47, 56	0
1	I	156/200 (78%)	-0.28	0	100	100	26, 32, 45, 56	0
1	J	155/200 (77%)	-0.20	0	100	100	30, 39, 54, 62	0
1	K	156/200 (78%)	-0.30	0	100	100	25, 32, 46, 66	0
1	L	155/200 (77%)	-0.08	2 (1%)	77	76	29, 38, 57, 64	0
All	All	1867/2400 (77%)	-0.26	5 (0%)	94	93	20, 30, 47, 66	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	13	ASN	2.7
1	L	30	VAL	2.6
1	G	168	LEU	2.3
1	L	35	ARG	2.1
1	F	168	LEU	2.1

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CL	A	201	1/1	0.98	0.36	35,35,35,35	0
2	CL	H	201	1/1	0.99	0.34	37,37,37,37	0

6.5 Other polymers (i)

There are no such residues in this entry.